

Disorder Induced Ferromagnetism in Restricted Geometries

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We study the influence of on-site disorder on the magnetic properties of the ground state of the infinite U Hubbard model for restricted geometries. We find that for two dimensional systems disorder enhances the spin polarization of the system. The tendency of disorder to enhance magnetism in the ground state may be relevant to recent experimental observations of spin polarized ground states in quantum dots and small metallic grains.

The interplay between disorder and interactions [1] and the possibility that it leads to ground state ferromagnetism has been the subject of much interest [2]. In several new experiments in restricted geometries, such as zero temperature transport measurements of the conductance through semiconducting quantum dots [3] and carbon nanotubes [4], tantalizing hints of a weakly ferromagnetic ground state of small systems with a few hundreds of electrons have appeared. The ground state spin polarization may be directly measured by coupling the dot or tube to external leads and measuring the differential conductance. Also from a recent mean field treatment of electron-electron interactions in disordered electronic systems [5] as well as from a numerical study of such systems [6] a partially magnetized ground state seems probable.

The canonical model for the study of itinerant ferromagnetism is the Hubbard model, described by the Hamiltonian

$$H = \sum_{i\sigma} \varepsilon_i n_{i\sigma} - t \sum_{\langle ij \rangle \sigma} a_{i\sigma}^\dagger a_{j\sigma} + c.c. + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $a_{i\sigma}^\dagger$ is the fermionic creation operator on site i with spin σ , $n_{i\uparrow} = a_{i\uparrow}^\dagger a_{i\uparrow}$, and the on-site energies ε_i are drawn randomly according to a uniform distribution between $-W/2$ and $W/2$. The large U regime of the model has attracted much interest due to its relevance to the theory of high- T_c superconductivity [7]. Although the model clearly does not contain many of the physical attributes of the typical experimental system such as a quantum dot (especially at the infinite U limit), nevertheless, it is important to gain insight into the complicated problem of the influence of disorder on the spin structure of interacting electrons in restricted geometries by studying simplified models. Moreover, the infinite U limit has the attractive feature of suppressing antiferromagnetic correlations which are clearly not relevant to quantum dots, even in the clean limit [8].

In this paper we study the effect of disorder on the enhancement of the spin polarizability of small interacting systems. For one dimensional infinite U Hubbard mod-

els, disorder does not essentially change the magnetization behavior [9]. On the other hand, for two dimensional systems, it is found that sufficiently strong disorder suppresses the singlet-favoring effects and the spin polarization of the system increases. From analytical arguments and numerical calculations it is shown that in the presence of disorder the fully polarized regime extends to higher densities of holes. Even beyond the fully polarized regime disorder creates a tendency towards non-zero magnetic moments in the ground state, which is consistent with other indications for such a behavior in disordered interacting systems.

The extensively studied Hubbard model, which is the simplest model of strongly correlated electrons, was originally introduced to explain ferromagnetism [11]. However, till now, little is known about the phase diagram of the model even at $T = 0$. There are a few rigorous results, mostly restricted to the one-dimensional model, or to the half-filled case. Lieb and Mattis have proven that for one dimensional systems (1D) for even number of electrons, with interaction strength $U < \infty$ and open boundary conditions (BC) [12] the ground state (GS) is a singlet. For higher dimensions and half filling it has been shown [13] that for a bipartite lattice with N_A (N_B) sites on sub-lattice A(B), the GS is non-degenerate and has total spin $\frac{1}{2}|N_A - N_B|$, as long as $U > 0$. In particular, for the square lattice, the GS is a singlet. In the large- U limit the problem is mapped onto the Heisenberg Hamiltonian, leading to antiferromagnetism (AFM) with long range order [14].

An important milestone in the research of ferromagnetism in Hubbard models is the work of Nagaoka [15]. It showed that for most lattices, with nearest-neighbor hopping and infinite on-site interaction U , the GS is the fully saturated ferromagnetic state, for the case of one hole in an otherwise half-filled band. An extensive work was done in order to find whether this result can be extended to higher hole density, or to finite U . It was shown that the two-hole case the GS is a singlet [16,17], but this GS is degenerate with the Nagaoka state in the thermodynamic limit. Various variational wavefunctions were

suggested to test the stability of the Nagaoka state (See [18–22] and references therein). Bounds were given to the holes density for which stability may remain. The best bound to date is $\delta_{cr} \leq 0.2514$ [20] (where δ is the number of holes per site). Still, the stability of the Nagaoka state, and the possibility of explaining ferromagnetism by it, is an unresolved problem [23].

In this letter we wish to show that in some sense the situation in the disordered case is simpler. Let us first sketch the situation in 1D. If periodic BC are imposed in 1D, the problem of m interacting electrons (at $U = \infty$) can be mapped onto a system of m non-interacting spinless fermions on 1D ring with fluxes $\Phi/\Phi_0 = 2\pi j/m$ ($j = 0, \dots, m-1$), where the GS energy corresponds to the flux j with the lowest energy [9]. This mapping shows that the effect of the spin background in 1D is trivial, and does not depend of the strength of disorder.

One might expect the effects of disorder in 2D to be smaller than in 1D, and thus no influence of disorder in 2D as well. However, the insensitivity of the 1D GS spin structure to disorder is accounted for by the fact that the spin permutation subgroup induced by the 1D hopping terms is cyclic [9]. Hence, spin background effects in 1D are not major. On the other hand, the permutation subgroup induced by the 2D hopping terms is non-abelian, and therefore the spin background has non trivial effects on the dynamics of the holes. Thus we might expect an interplay between disorder and the behavior of the spin background in 2D.

We start by considering the influence of disorder on the one hole case. The hopping of the hole around the lattice induces permutations in the spin ordering. The hopping term is then effectively reduced by a factor proportional to the expectation value of the different permutations. In order to minimize kinetic energy, this overlap should be maximal, and this is achieved by the fully polarized state for which the spin wavefunction is unchanged by permutations of different spins. This argument does not change due to disorder, and it leads to the Nagaoka's theorem which assures us that the GS is fully polarized, even in the presence of disorder.

The two holes case is much more complicated. Although the above argument for preferring the FM order applies for the case of several holes equally, it is known that in the ordered case the GS is a singlet [16,17]. This is accounted for by the re-ordering of the spin background in order to mask the fermionic BC between the holes. Thus, the spin background takes care for the anti-symmetrization of the many body (in fact, many-holes) wave function, and thus the spatial function has less nodes, which decrease its energy. It was shown, for a special variational wave function, that the resulting energy gain supersedes the energy increase at the bottom of the band, coming from the reduction of the hopping amplitude due to the Nagaoka effect [16]. Thus, the tendency towards ferromagnetism is suppressed, and the

spin structure, if any, is of a much more complex form [10].

As disorder increases, the single particle functions become more and more localized (in the participation ratio sense). The overlap of the different single particle functions decreases, and thus, the fermionic BC constraint (i.e., a zero of the many body wavefunction wherever two particles are on the same site) becomes less restrictive, and does not change the many body energy much. Therefore, one may expect that the incentive for re-ordering of the spin background decreases, while, as in the one hole case, there still is a contribution from the hopping amplitude leading to a Nagaoka state.

Exact diagonalization for the full many-particle Hamiltonian of Eq. (1) was used to test the above arguments. Although we have used small systems one may expect that due to the chaotic nature of the dots [6] the dependence on the number of electrons or the BC will play a less important role for disordered systems than in clean ones [10]. Thus, the study of a small number of electrons is still useful in understanding the properties of dots which are populated by an order of magnitude more electrons. We have used up to 14 electrons on up to 4×4 lattices. The size of the Hilbert space is then 471435600, which is far beyond exact diagonalization capabilities. Fortunately one can omit the double occupied states for $U = \infty$ and use the spin symmetry of the Hamiltonian to reduce this number considerably. The number of spatial functions in this case is 120, and the number of total spin configurations in the $S_z = 0$ sector is 3432, yielding a total of 411840 states. We have used group theory to construct the definite S states, and to decompose the space into subspaces of definite S and S_z . The largest sectors ($S = 1, 2$) consisted of 1001 spin functions and a total of 120120 basis functions. Group theory was used for constructing the matrices describing the effect of hopping on the different spin functions. We then employed the Lanczos algorithm to find the exact GS for 600 realizations at every disorder value. In the ordered case, the GS was a singlet, in accordance with [16,17]. Figure 1 presents the GS-spin distributions as a function of W , for 14 electrons on a hard-wall 4×4 lattice. The average spin $\langle S \rangle$ is also plotted against W , and one can see that it increases significantly with W . In the presence of disorder, one gets a distribution of GS-spin values. For weak disorder, the main effect is smearing the peak at $S = 0$ to low S values. Thus, a tendency towards weak ferromagnetism is clearly demonstrated even for weak disorder ($W = 3t$) which corresponds to a ballistic (mean free path larger than the system size) regime. Moreover, as disorder increases, high S values dominate the distribution. For $W = 6t$ corresponding to a diffusive regime a clear dominance of the high spin state appears.

Similar behavior was obtained for smaller lattices and periodic BC. Fig. 2 presents the results for the same conditions as in Fig. 1 employing periodic BC. Clearly,

the tendency towards ferromagnetic behavior persists, although higher values of W needed to obtain similar values of spin polarization. This is the result of the fact that for periodic BC, higher values of W are needed to generate the same value of dimensionless conductance. One sees that, in contrast with the situation in the ordered case, our results are not sensitive to the lattice size or the BC. This manifests the chaotic nature of the dot, which suppress dependencies on the details of the system.

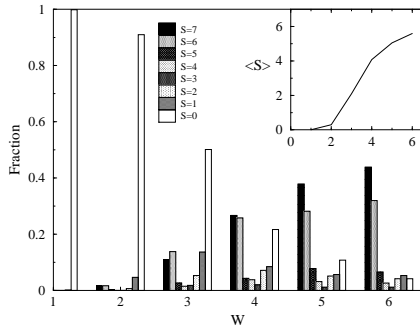


FIG. 1. The spin distributions as a function of disorder W for a 4×4 lattice with 14 electrons. For each W , the bar chart represents the probability of finding the GS of the system at a particular value of S . The inset presents the average spin $\langle S \rangle$ as a function of W .

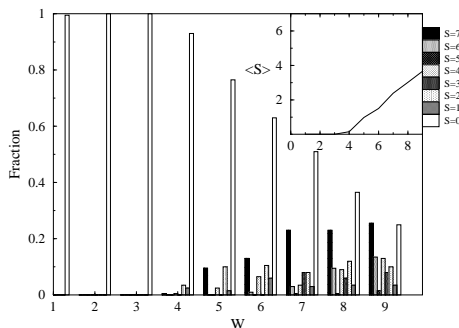


FIG. 2. Same as Fig. 1 for periodic BC.

A clear manifestation of this point is presented by the results for 13 electrons on a 5×3 lattice. In the ordered case, the behavior of this cluster depends dramatically on the BC. For hard-wall BC, the GS is fully polarized (i.e., $S = 13/2$), while for periodic BC, the GS has the minimal spin $S = 1/2$. On the other hand, once the system is diffusive the GS-spin polarization distributions become closer and when the dimensionless conductance

is of order one, both distributions are quite similar, where $\langle S \rangle = 5.90$ for hard-wall BC and $\langle S \rangle = 3.96$ for periodic BC.

Exact diagonalization also confirms the tendency towards non-zero ground state spin values even for a higher number of holes. In Fig. 3 we depict the spin distribution for 12 electrons on a hard-wall 5×3 lattice (3 holes). The GS-spin is significantly enhanced as function of disorder, although the most probable spin state is not fully ferromagnetic. This tendency towards partial polarization of the ground state persists in higher hole ratios.

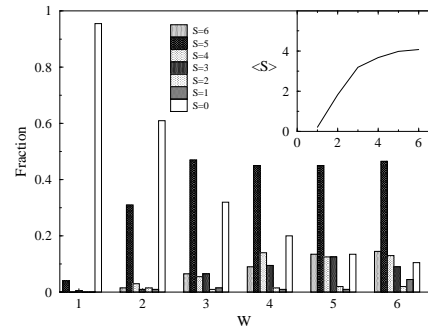


FIG. 3. The spin distributions as a function of disorder W for a 5×3 lattice with 12 electrons.

The method of exact diagonalization is restricted to small lattices. In order to learn whether the tendency towards ferromagnetism persists for larger systems we turn to a variational method. Many authors have considered various variational wave functions to study the instability of the Nagaoka state of the $U = \infty$ model for a thermodynamic concentration of holes [18–22]. Since the reliability of these functions for an accurate calculation of the phase boundary of ferromagnetism is doubtful, we only use this method to get a hint about disorder influence of the stability. For this purpose, we use the most simple of these functions [18], which is one of a single particle excitation. An up spin electron is removed from the occupied states and placed with flipped spin into another state. Direct calculation of the excitation energy in the ordered case [18] yields stability of the Nagaoka state with respect to spin flip for $\delta = 0.49$ (for a square lattice), while for smaller hole concentration, the Nagaoka state remains stable with respect to this excitation. We have done the calculation for the disordered case by taking different realizations of disorder of a 24×24 system, diagonalizing the single particle (non-interacting) Hamiltonian to find its eigenvalues and eigenvectors, and then calculating directly the excitation energy of the single flip variational wave function. Figure 4 shows the stability regime in the $\delta - W$ plane, as follows from this excitation calculation. For an ordered system we get the result of Ref. [18]

that the ferromagnetic state is stable for $\delta \leq 0.49$. However, as disorder increases, the stability regime grows. It therefore seems that the exact results for small systems characterize the behavior in larger systems as well. We note that analytical calculation of the excitation energy in the disordered case according to random vector model (RVM) yields a completely different behavior. This stems from the fact that RVM ignores correlations between the wavefunctions and the eigenvalues which are important in this case.

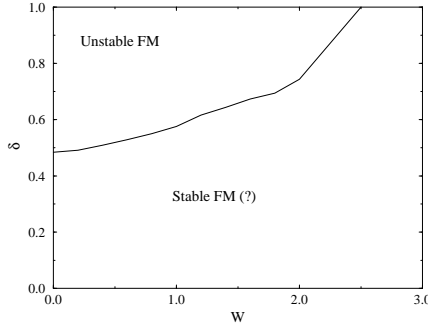


FIG. 4. Stability curve for the single flip excitation: the critical hole density δ vs. the disorder distribution width W

We would like to add a remark about the $U = \infty$ limit. The Nagaoka's effect and the decrease in the singlet favoring effect described here, are not unique to the $U = \infty$ limit. However, for the Hubbard model, ferromagnetism arises (even for one hole) only for $U \gg t$. The reason is that due to the perfect nesting property of the lattice model, the GS of the almost half filled case tends to be AFM. In order to wash out this tendency, the limit $U = \infty$ is taken. However, in reality, quantum dots do not show AFM behavior, since they are not described by a perfect lattice. One then might expect the previously described effect, namely the formation of larger magnetic moments due to disorder, to show in real quantum dots even for moderate values of U .

In conclusion, the influence of disorder on the magnetic properties of the GS was studied. For an ordered system, large magnetic moments are generally suppressed, and the spin structure of the GS, if any, is very complicated. On the other hand, we have shown that disorder plays an important role in determining the spin polarization of 2D systems described by the infinite U Hubbard model. Weak disorder tends to create a partially polarized ground state, while stronger disorder tends to stabilize a fully ferromagnetic GS. This behavior clearly indicates that there is a basis to expect that for more realistic descriptions of the experimental systems ($U \neq \infty$) disorder will play an important role in creating a spin polarized ground state.

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